201-15143

HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

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TEST PLAN

For

Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide

CAS No. 80-51-3

Submitted to the US EPA

By

Crompton Corporation

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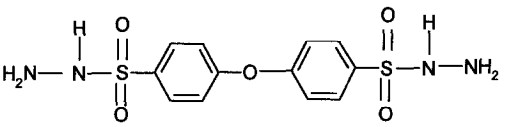
Test Plan for 4,4'-oxydibenzenesulfonohydrazide

1. General Information

1.1 CAS Number: 80-51-3

1.2 Molecular Weight: 358.39

1.3 Structure and formula: $C_{12}H_{14}N_4O_5S_2$



1.4 Introduction

Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide is used as a chemical blowing agent in the manufacture of foam rubber and plastic products.

2. Review of Existing Data and Development of Test Plan

Crompton Corporation has undertaken a comprehensive evaluation of all relevant data on the SIDS endpoints of concern for Celogen OT. The availability of the data on the specific SIDS endpoints is summarized in Table 1. Table 1 also shows data gaps that will be filled by additional testing.

Table 1: Available adequate data and proposed testing for Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide

CAS No. 80-51-3	Information	GLP	OECD Study?	Other Study?	Estimation Method?	Acceptable?	SIDS Testing required?
	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
Physicochemical							
Melting Point	Y	N			N	Y	N
Boiling Point	Y	N			N	Y	N
Vapour Pressure	Y	N			Y	Y	N
Water Solubility	Y	N			Y	N	Y
Partition Coefficient (Kow)	Y	N			Y	Y	N
Environmental Fate							
Biodegradation	Y				Y	N	Y
Hydrolysis	N						N
Photodegradation	Y				Y	Y	N
Transport and Distribution between Environmental Compartments	Y				Y	Y	N
Ecotoxicology							
Acute Fish	Y				Y	N	Y
Acute Daphnia	Y				Y	N	Y
Acute Algae	Y				Y	N	Y
Toxicology							
Acute Oral	Y	N		Y		Y	N
Repeat Dose toxicity	Y	N			N	N	Y
Genetic toxicity – Gene mutation	Y	N			N	N	Y
Genetic toxicity – Chromosome aberration	Y				N	N	Y
Reproductive toxicity	N						Y
Developmental toxicity/teratogenicity	N						Y

A. Evaluation of Existing Physicochemical Data and Proposed Testing

1. Melting Point

It is reported in a peer-reviewed publication that Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide begins to decompose at 150-160°C prior to melting.

2. Boiling Point

The boiling point of Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide cannot be measured as the substance decomposes prior to melting.

3. Vapour Pressure

The vapour pressure of Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide was calculated to be $8.9x10^{-12}$ hPa at 25°C using MPBPWIN v1.40.

4. Water Solubility

A water solubility study will be conducted following OECD guidelines.

5. Partition Coefficient

The log Pow of Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide was estimated to be 0.08 using KOWWIN v1.66.

Summary of Physicochemical Properties Testing: Existing data for melting point, boiling point, vapour pressure and partition coefficient are considered to fill these endpoints adequately . A water solubility test will be conducted.

B. Evaluation of Existing Environmental Fate Data and Proposed Testing

1. Biodegradation

A Biodegradation study will be conducted following OECD guidelines.

2. Hydrolysis

There are no hydrolysable groups in the chemical structure, and the substance is therefore predicted to be hydrolytically stable.

3. Photodegradation

The potential for photodegradation of Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide has been estimated using AOPWIN v1.90, and indicated atmospheric oxidation via OH radicals reaction with a half-life of 61 hours.

4. Transport and Distribution between Environmental Compartments

An Epiwin Level III Fugacity Model calculation has been conducted for Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide and indicates even distribution between soil and water for emissions of 1000 kg/hr simultaneously to air, water and soil compartments. . The

fugacity model estimates will be recalculated once measured data on the water solubility is available.

Summary of Environmental Fate Testing: Existing data for photodegradation and transport and distribution between environmental compartments are considered to fill these endpoints adequately. A Biodegradation study will be conducted.

C. Evaluation of Existing Ecotoxicity Data and Proposed Testing

1. Acute Toxicity to Fish

An Acute toxicity to Fish study will be conducted following OECD guidelines.

2. Acute Toxicity to Algae

An Acute toxicity to Algae study will be conducted following OECD guidelines.

3. Acute Toxicity to Daphnia

An Acute toxicity to Daphnia study will be conducted following OECD guidelines.

Acute toxicity to Fish. Daphnia and Algae studies.will be conducted following OECD guidelines.

D. Evaluation of Existing Human Health Effects Data and Proposed Testing

1. Acute Toxicity

The acute oral toxicity has been determined to be > 5200 mg/kg b.w. The acute dermal toxicity has been determined to be > 200 mg/kg b.w. (FIFRA Section 162.8(c)). When administered by interperitoneal injection, a LD_{50} >5000 mg/kg b.w. was observed. No further data on purity of the test material, tested doses, and systemic toxicity in target organs by dose and sex are available.

2. Skin Irritation

This non-SIDS endpoint has been evaluated for Celogen OT. Slight irritation occurred in rabbits treated with an aqueous extract of the chemical.

3. Repeat Dose Toxicity

Two repeat dose toxicity studies are reported in the literature. In the first of these a NOEL of 1mg/kg bw/day (90 day, oral feed, rat) was reported. In the second study a LOAEL of 36 mg/kg/day (4 month, gavage, rat) was reported. A combined repeat dose/reproductive/developmental toxicity screening test will be determined using OECD Method 422

4. Genotoxicity

The substance was mutagenic in the Ames test (S. typhimurium) with and without metabolic activation and also with one strain of Escherichia coli with metabolic activation. With other strains of E. coli, the substance was found to be non-mutagenic with or without metabolic activation. The substance gave negative results in a chromosome aberration study using human lymphocytes. It also gave negative results in a micronucleus assay and UDS assay. However there is insufficient information to assess the reliability of the results. Genetic toxicity studies will be conducted following OECD guidelines.

5. Reproductive and Developmental Toxicity

A combined repeat dose/reproductive/developmental toxicity screening test will be determined using OECD Method 422.

Summary of Human Health Effects Testing: Genotoxicity and a

3. Evaluation of Data for Quality and Acceptability

The collected data were reviewed for quality and acceptability following the general US EPA guidance [2] and the systematic approach described by Klimisch et al [3]. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to ecotoxicology and human health endpoint studies per EPA recommendation [4]. The codification described by Klimisch specifies four categories of reliability for describing data adequacy. These are:

(1) Reliable without restriction: Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.

(2) Reliable with Restrictions: Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.

(3) Not Reliable: Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

(4) Not Assignable: Includes studies or data in which insufficient detail is reported to assign a rating, e.g. listed in abstracts or secondary literature.

4. References

[1] US EPA, EPI Suite Software, 2000

[2] USEPA (1998). Guidance for Meeting the SIDS Requirements (The SIDS Guide). Guidance for the HPV Challenge Program. Dated 11/2/98.

[3] Klimisch, H.-J., et al (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5

[4] USEPA (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 2/10/99.